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Kondo hole in one-dimensional Kondo insulators

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Properties of a non-magnetic impurity in Kondo insulators are investigated by considering a one-dimensional Kondo lattice model with depletion of a localized spin. The ground state phase diagram determined by the Lanczos method shows that the magnetic moment is more stable than in ordinary metals. Temperature dependence of impurity susceptibilities is also studied by using the finite temperature density-matrix renormalization group.

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I. INTRODUCTION

The single-impurity Anderson model [1] was introduced to study the condition for formation of localized moments in metals. The self-consistent Hartree-Fock method showed that there is a transition between the magnetic state and the non-magnetic state at $U_c \sim 1/\rho_d$, where U is on-site Coulomb energy of a virtual bound state, and ρ_d is its density of states at the Fermi level. But as a result of the Kondo effect [2], the sharp transition disappears and becomes a cross-over. That is, at high temperatures higher than the Kondo temperature, there is the region where thermodynamic properties are well described by the localized magnetic moment. At zero temperature, however, the magnetic moment disappears by the Kondo effect leading to the singlet ground state which is obtained by K.Yosida [3].

In metals, gap-less excitations around the Fermi energy play an important role to the Kondo effect. On the contrary, in spin-1/2 anti-ferromagnetic (AF) Heisenberg two-leg ladders, which have spin gaps and short range singlet correlations, a non-magnetic impurity, *i.e.* depletion of a spin, induces a local magnetic moment around the vacant site because the impurity breaks a dimer singlet pair of the resonating valence bond (RVB) state and leaves an unpaired spin [4, 5]. In fact, the magnetic moments exhibit a Curie law susceptibility, whose Curie constant is proportional to the concentration of the impurities [6]. Correlations between the magnetic moments are staggered and rapidly decaying with the impurity distance. Experimentally, when concentration of the impurities exceeds a critical value, the spin gap disappears and it leads to an instability of the spin-liquid state towards an AF ordered state [7]. On the other hand, theoretically, the critical concentration seems to be zero for a bipartite lattice and thus any finite concentration of impurities leads to the ground state with AF quasi long range order and gap-less excitations.

An impurity in the Kondo Lattice (KL) model which describes heavy fermion system is introduced as a depletion of a localized spin similarly to the impurities in the two-leg spin ladder. However, since the KL model includes both itinerant electrons and localized spins in contrast to the spin ladder systems, after the depletion one should ask necessary condition for formation of the localized moment on the impurity site. The model Hamiltonian for general dimension d is defined as

$$
\begin{aligned}
H &= \sum_{\langle n,n'\rangle,s} t_{n,n'} c^\dagger_{ns} c_{n's} + J \sum_{n\neq n_d} \mathbf{S}_n \cdot \mathbf{s}_n \\
&\quad + \epsilon \sum_s c^\dagger_{n_d s} c_{n_d s} + U c^\dagger_{n_d\uparrow} c_{n_d\uparrow} c^\dagger_{n_d\downarrow} c_{n_d\downarrow}, \qquad (1)
\end{aligned}
$$

where $\mathbf{s}_n := \sum_{s,s'} \frac{1}{2}\sigma_{s,s'} c^\dagger_{ns} c_{ns'}$ and n is d-dimensional vector and n_d indicates the impurity site. This model represents a single impurity and the surrounding KL model. It can be viewed also as the KL model without the spin at $n = n_d$: the KL model with a Kondo hole. When the KL model at half filling, so-called Kondo insulator, is considered we may expect that the existence of a spin gap and a charge gap will lead to similar properties as the two-leg spin ladder in certain situations. In fact, by substituting non-magnetic Lu-ions into a Kondo insulator, $Yb_{1-x}Lu_xB_{12}$, Curie-like susceptibilities are observed at low temperatures for small concentrations [8]. This fact suggests that localized magnetic moments are induced by the substitution of the non-magnetic Lu-ions. Correspondingly, the optical gap of the Kondo insulator YbB_{12}, is partially filled by the substitution [9].

Formation of impurity bands in Kondo insulators is discussed by Schlottmann and his coworker by using the periodic Anderson model by employing the $1/d$ expansion for the self-energy of the host sites for which the second order perturbation is used [10]. Concerning the impurity site, Coulomb interaction is neglected, corresponding to $\epsilon = U = 0$ in our notation.

In this paper, we study the condition for the presence or absence of localized moments in Kondo insulators and properties of these moments. For this purpose, we will restrict ourselves to the one-dimensional (1D) case (Fig. 1), setting the hopping parameter $t_{n,n'} = -t = -1$ (*i.e.*, measuring all energies in units of t). In the one-dimension we can use various powerful methods like the numerical exact diagonalization and the density matrix renormal-

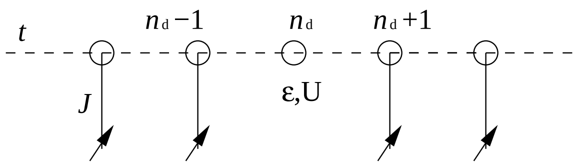

FIG. 1: The one-dimensional Kondo lattice model with an impurity site, n_d.

ization group. Various properties of the pure 1D Kondo insulator:

$$H_{\rm KL} = \sum_{\langle n,n' \rangle, s} t_{n,n'} c^{\dagger}_{ns} c_{n's} + J \sum_{n} \mathbf{S}_n \cdot \mathbf{s}_n \tag{2}$$

have been studied extensively [11]. In particular, magnitudes of the charge gap and the spin gap are obtained numerically [12]. The spin-spin correlation functions decay with oscillations, the RKKY oscillations, and its correlation length ξ are also determined [13].

II. PROPERTY OF THE GROUND STATE

In order to determine the magnetic or non-magnetic ground state, the total number of conduction electrons $N_{\rm tot}$ and the total spin $S^z_{\rm tot}$ are studied. Since the surrounding Kondo insulator has the totally singlet ground state when the impurity site is neglected, we expect that there is one-to-one correspondence between $N_{\rm tot}$ and the existence or absence of the magnetic moment around the impurity site. Let us start from the strong coupling limit, $J/t \gg 1$. To make the following discussion clear we assume a finite J and $t = 0$. Then the impurity site is independent from the rest and it is sufficient to think only four states for the impurity site: the unoccupied impurity state ($S^z_{\rm tot} = 0, N_{\rm tot} = L-1$), the doublet ($S^z_{\rm tot} = \pm\frac{1}{2}, N_{\rm tot} = L$), and the doubly occupied state ($S^z_{\rm tot} = 0, N_{\rm tot} = L+1$), where L is the number of the lattice sites including the impurity site. In this case, it is clear that these states are distinguished with the total number of conduction electrons of the ground state $\langle N_{\rm tot} \rangle_{\rm gs}$. For a finite t various hopping processes take place. However, these processes keep the number of conduction electrons and total spin of the system. Since the quantum numbers mentioned above define a disjoint subspace, we can investigate the problem of formation of magnetic moment just by looking at the total number of electrons at finite J/t. The quantum number of the ground state is obtained by comparing the lowest eigenvalues with the Lanczos method for different submatrices. We place the impurity site at the center and use the open boundary conditions.

There is an electron-hole symmetry for the present system. By using the transformation, $c_{ns} \to (-1)^n c^{\dagger}_{ns}$ and

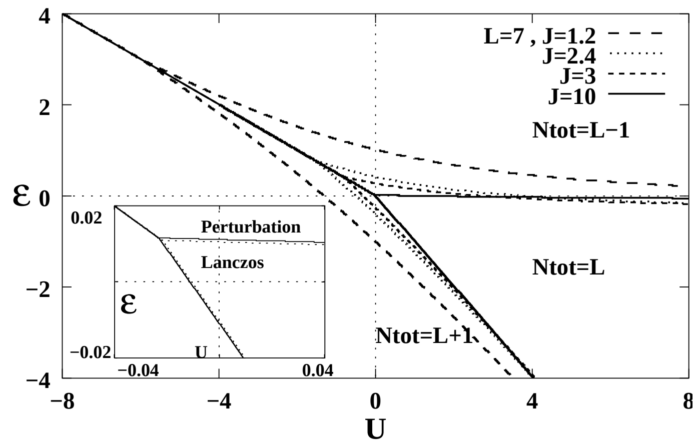

FIG. 2: Phase diagram of $\langle N_{\rm tot} \rangle_{\rm gs}(U,\epsilon)$ obtained from the Lanczos method using the same $L = 7$ for $J = 1.2, 2.4, 3, 10$. Inset:comparison between the results by the Lanczos method (dashed lines) and the fourth order t/J perturbation (solid lines) for $J = 10$.

$\mathbf{S}_n \to -\mathbf{S}_n$, the Hamiltonian (Eq. 1) is reduced to

$$\begin{aligned} H' &= \sum_{\langle n,n' \rangle, s} t_{n,n'} c^{\dagger}_{ns} c_{n's} + J \sum_{n \neq n_d} \mathbf{S}_n \cdot \mathbf{s}_n \\ &\quad -(\epsilon + U) \sum_{s} c^{\dagger}_{n_d s} c_{n_d s} + U c^{\dagger}_{n_d \uparrow} c_{n_d \uparrow} c^{\dagger}_{n_d \downarrow} c_{n_d \downarrow} \\ &\quad +2\epsilon + U, \end{aligned} \tag{3}$$

where the last term $2\epsilon + U$ can be ignored. Therefore the physical properties for a set of parameters (U, ϵ) are identical to the system with $(U, -\epsilon - U)$. In particular, since n_{ns} goes to $1 - n_{ns}$ under the transformation, this symmetry leads to

$$\langle N_{\rm tot} \rangle_{\rm gs}(U,\epsilon) = 2L - \langle N_{\rm tot} \rangle_{\rm gs}(U, -\epsilon - U). \tag{4}$$

In the strong coupling limit ,$J = \infty$, the energies of $N_{\rm tot} = L-1, L, L+1$ are determined as $0, \epsilon, 2\epsilon + U$. In particular when $\epsilon = U = 0$, these three states are degenerated. We define such a point as the tricritical point (U_c, ϵ_c) (*i.e.*, $(U_c, \epsilon_c) = (0, 0)$ at $J = \infty$). In general, from the electron-hole symmetry one can show that the tricritical point (U_c, ϵ_c), if it exists, must be on the symmetric line $\epsilon_c = -U_c/2$.

Figure 2 shows that as decreasing J, the domain of the doublet $\langle N_{\rm tot} \rangle_{\rm gs}(U,\epsilon) = L$ (*i.e.*, the magnetic state) is extended. The transition lines of $J = 10$ (the solid lines in Fig. 2) are very close to those of the strong coupling limit. In the strong coupling case, $J/t \gg 1$, one can use the perturbation theory to estimate the boundaries. In the inset of Fig. 2, comparison is made between the fourth order perturbation results and the numerical ones for $J = 10$. The agreement is satisfactory.

We comment on the finite-size effect on the phase diagram. The numerical results shown in Fig. 2 are for a fixed system size, $L = 7$. When $J \geq 2.4$, the system-size dependence of $\langle N_{\rm tot} \rangle_{\rm gs}(U,\epsilon)$ is very small and

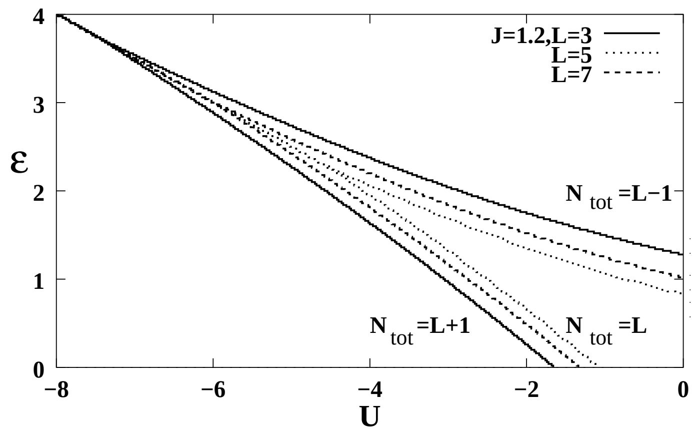

FIG. 3: The finite size effect on the phase diagram obtained from the Lanczos method for $J = 1.2, t = 1$ with varying $L = 3, 5, 7$.

J	U_c
1.2	-5.96 < U_c < -4.54
2.4	-1.58 ±0.02
3	-0.82 ±0.02
∞	0

TABLE I: Tricritical point $U_c(J)$ estimated from the Lanczos method. ϵ_c is given by $-U_c/2$.

has reached a convergence within $L < 7$. But, when J becomes smaller the system-size dependence becomes more significant. Fortunately, however, the finite-size effect shows an alternating behavior as shown in Fig. 3. From the system-size dependence, we may conclude that $-5.96 < U_c < -4.54$ for $J = 1.2$. Table I summarizes the results of the tricritical points for various J, where the errors are estimated from the finite-size effect.

III. TEMPERATURE DEPENDENCE OF SUSCEPTIBILITIES

In order to study the process of formation of the magnetic moment as a function of temperature, we calculate susceptibilities. The values of susceptibilities at zero temperature depend on the nature of the ground state. At low temperatures, susceptibilities diverge like a Curie-law if the ground state is magnetic, while converge to zero if the ground state is non-magnetic.

1. *definition of susceptibilities*

With a global magnetic field h, we define total and impurity susceptibilities in the following way,

$$\chi_{\rm tot} \;:=\; \frac{\partial \langle S^z_{\rm tot}\rangle}{\partial h}, \tag{5}$$

$$\chi_{\rm imp} \;:=\; \frac{\partial \langle s^z_{n_d}\rangle}{\partial h}, \tag{6}$$

where the z-component of the total spin is given by $S^z_{\rm tot} := \left(\sum_{n\neq n_d} S^z_n + \sum_n s^z_n\right)$. The system consists of the $L-1$ sites of the Kondo insulator and one impurity site. Therefore, in order to extract the impurity effect, we define another impurity susceptibility:

$$\chi_d \;:=\; \chi_{\rm tot} - \frac{L-1}{L}\chi^{\rm KL}_{\rm tot}, \tag{7}$$

where $\chi^{\rm KL}_{\rm tot}$ is defined by $\chi_{\rm tot}$ of the 1D Kondo insulator without any impurity (Eq. 2). Of course, the contributions to this susceptibility from the Kondo insulator parts are zero at zero temperature, because both of them have the singlet ground states.

These susceptibilities are calculated by using the finite-temperature density-matrix renormalization group (finite-T DMRG) [14] method as follows. From the maximum eigenvalue λ_M of the quantum transfer matrix $\mathcal{T}_M$, the partition function $Z_{\rm KL}$ of the 1D Kondo insulator without any impurity (Eq. 2) is given by

$$\begin{aligned} Z_{\rm KL} \;&=\; {\rm tr} e^{-\beta H_{\rm KL}} = \lim_{M\to\infty} {\rm tr}\mathcal{T}_M{}^{L/2} \\ &=\; \lim_{M\to\infty} \lambda_M^{L/2},\ \text{when } L\to\infty, \end{aligned} \tag{8}$$

where M is the Trotter number. The last equality is obtained in the thermodynamic limit $L\to\infty$. Following S.Rommer [15], we obtain the partition function Z of the model Hamiltonian (Eq.1) by the quantum transfer matrix of the impurity site $\mathcal{T}^{\rm imp}_M$.

$$\begin{aligned} Z \;&=\; {\rm tr} e^{-\beta H} = \lim_{M\to\infty} {\rm tr}\mathcal{T}_M{}^{L/2-1}\mathcal{T}^{\rm imp}_M \\ &=\; \lim_{M\to\infty} \lambda_M^{L/2-1}\langle \Psi^{\rm L}_M|\mathcal{T}^{\rm imp}_M|\Psi^{\rm R}_M\rangle,\ \text{when } L\to\infty, \end{aligned} \tag{9}$$

where λ_M and the normalized eigenvectors $\langle\Psi^{\rm L}_M|, |\Psi^{\rm R}_M\rangle$ are obtained from the finite-T DMRG for a given trotter number M. The susceptibility is obtained from the free energy F or the magnetization m numerically as $-\delta F/\frac{\delta h^2}{2}$ or $\delta m/\delta h$ under a small magnetic field δh. Typical truncation errors in the infinite-system algorithm of finite-T DMRG method are 10^{-2} at the lowest temperature $kT = 0.12$ for the Trotter number $M = 200$.

In addition, non-local susceptibilities can be defined by applying a small magnetic field on a site, for example at the impurity site, and measure magnetization at different sites. We will use such susceptibilities in latter discussions to investigate how effects of the impurity moment extend to the bulk of the Kondo insulators.

2. Result of susceptibilities

In the strong coupling limit, $J = \infty$, it is simple to calculate the susceptibilities, because the magnetic moment is completely localized at the impurity site: $\chi^{(0)}_{\rm tot} = (L-1)\beta\frac{1+2e^{-J\beta/3}}{e^{3J\beta/4}+4+e^{-J\beta/3}} + \chi^{(0)}_{\rm imp}$, $\chi^{(0)}_{\rm imp} = \chi^{(0)}_d = \beta\frac{1}{2(2+e^{\beta\epsilon}+e^{-\beta(\epsilon+U)})}$. These susceptibilities at low temperatures show a sharp transition at the boundaries around the magnetic solution. In the magnetic region, the ratio of the susceptibilities to the Curie law susceptibility ($\chi_{\rm C} = 1/4kT$) converge to unity in the limit of $T \to 0$: $\chi^{(0)}_{\rm imp}/\chi_{\rm C} = \chi^{(0)}_d/\chi_{\rm C} = 1$.

At high temperatures $T \gg J$ and t , susceptibilities of any J/t show good agreement with the susceptibilities of the strong coupling limit, since correlations between different sites are negligible. In fact, the high-temperature expansion of the susceptibility χ, which is obtained from the second order perturbation of t/J, is given by $\chi_{\rm imp} - \chi^{(0)}_{\rm imp} = -t^2\beta^3/4$.

On the other hand, at low temperatures the values of susceptibilities depend on the ground state as we mentioned at the beginning of this section. Figure 4 shows $\chi_d/\chi_{\rm C}$ for various J and (U, ϵ) on the symmetric line: $U = 8, 0, -8$ and $\epsilon = -U/2$. First we note that $\chi_d/\chi_{\rm C}$ for $U = 0$ and $J = \infty$ is special and temperature independent. This is due to the fact that $U = 0$ and $\epsilon = 0$ is the tricritical point in the strong coupling limit. Except for $U = 0$ and $\epsilon = 0$ case, all lines are pointing towards either zero or unity in the zero temperature limit. These behaviors are consistent with the values of the tricritical point in Table I estimated from the ground state. However the temperature dependence of $\chi_d/\chi_{\rm C}$ is quite different for $U = 8$ and 0.

To understand the difference, we plot $\chi_{\rm imp}/\chi_{\rm C}$ in Fig. 5. One can see that $\chi_{\rm imp}/\chi_{\rm C}$ approaches to a finite value for $U = 8$ and 0 while it goes to zero for $U = -8$. Furthermore the finite value seems to depend on U and$J$. As can be seen from the definition of $\chi_{\rm imp}$ (Eq. 6), only the induced moment at the impurity site is measured for this susceptibility, while the entire moment induced in the system is measured for χ_d (Eq. 7). Therefore the different limit $\chi_{\rm imp}/\chi_{\rm C}$ may be understood as due to the difference in the spatial spread of the induced magnetic moment. Naturally, we expect that the induced moment has a larger amplitude at the impurity site for larger U ($> U_c$) and a wider spread for smaller J since the correlation length of the Kondo insulator gets longer as J is decreased [13]. We may conclude that the limiting value of $\chi_{\rm imp}/\chi_{\rm C}$ is larger for larger U ($> U_c$) and larger J. This is exactly what we observe in Fig. 5

In order to investigate spatial spread of the magnetic moment, we calculate the susceptibilities

$$\chi_{s_n} \;:=\; \frac{\delta\langle s^z_n\rangle}{\delta h_d}, \tag{10}$$

where h_d is the local magnetic field applied on the impurity site only.

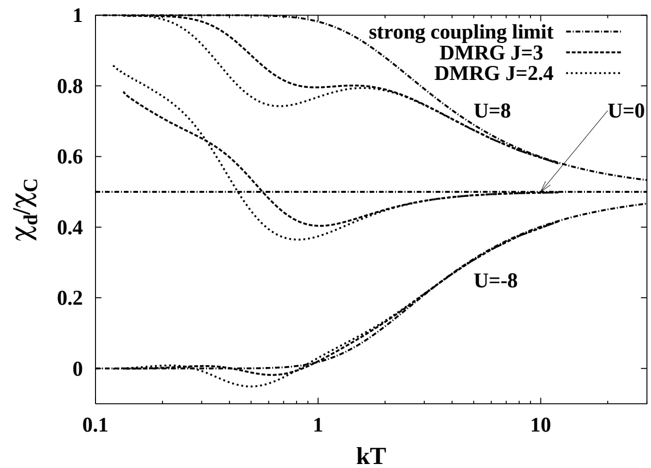

FIG. 4: Ratio of the susceptibility χ_d to the Curie susceptibility $1/4kT$ calculated by the finite-T DMRG method for $J = 3, 2.4$ and for $\epsilon = -U/2$; $U = 8, 0, -8$.

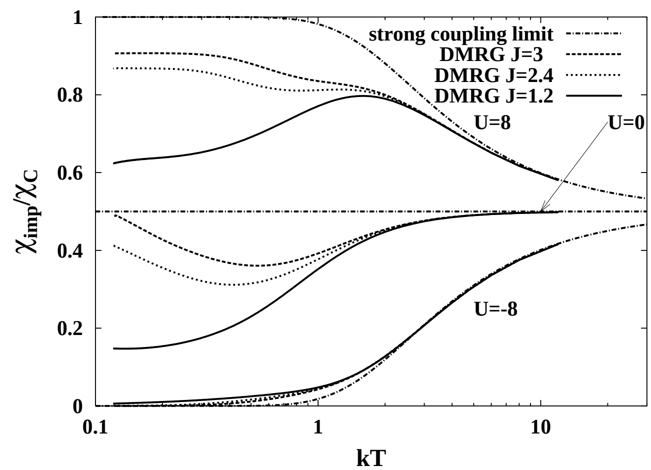

FIG. 5: Ratio of the susceptibility $\chi_{\rm imp}$ to the Curie susceptibility $1/4kT$ calculated by the finite-T DMRG method for $J = 3, 2.4, 1.2$ and for $\epsilon = -U/2$; $U = 8, 0, -8$.

When a magnetic field is applied on one site in the Kondo lattice model, the induced magnetic moments show the RKKY oscillatory behavior

$$\langle s_n\rangle \;\propto\; (-1)^{(n-n_0)}\exp(-|n-n_0|/\xi), \tag{11}$$

where ξ is the correlation length. Thus we expect that the non-local susceptibilities χ_{s_n} also show a similar behavior.

It is interesting to estimate the correlation length from the ratio between $\chi_{s_{n_d+1}}$ and $\chi_{s_{n_d}}$ through the relation

$$\xi^{-1} \;=\; -\log(-\chi_{s_{n_d+1}}/\chi_{s_{n_d}}). \tag{12}$$

Figure 6 shows that values of ξ at low temperatures estimated from the above relation are close to the correlation length of the 1D Kondo insulator evaluated at $T = 0$ by

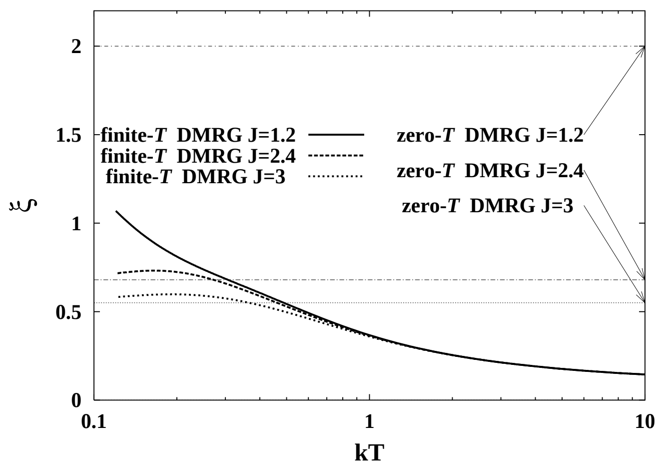

FIG. 6: The correlation length ξ estimated from $\chi_{s_{n_d}}$ and $\chi_{s_{n_d+1}}$ for $J = 1.2, 2.4, 3$. The correlation lengths of the bulk Kondo insulator obtained by the zero-temperature DMRG method [13] are also shown.

the zero-temperature DMRG [13]. The value of ξ increases with decreasing J, which is consistent with the divergence of the correlation length at $J = 0$ [13].

Finally we would like to comment on the non-monotonic temperature dependence observed in Fig. 4. The decrease of the ratio of the susceptibility to the Curie susceptibility around $T = 2$ with lowering temperature is due to formation of conduction band. This is a general trend which is shown by the above second order perturbation theory with respect to t/J. On the other hand, the upturn around $T = 0.5 \sim 0.8$ may be traced back to the effect of formation of the Kondo singlet states on both sides of the impurity. In fact, this idea is consistent with the fact that the minimum occurs around the spin gap temperature of the Kondo insulators, however, further investigation is necessary to draw a definitive conclusion.

IV. CONCLUSIONS

In this paper we have studied the problem of formation of magnetic moment when a Kondo insulator is doped with an impurity without the localized spin. One dimensional Kondo lattice or Kondo chain is treated in this article. The ground state phase diagram is obtained by the Lanczos method. Temperature dependence of the impurity susceptibilities calculated by the finite-T DMRG are consistent with the phase diagram.

In contrast to the naive expectation, the region of stable magnetic moment in the (U, ϵ) plane is wider for smaller J. It is surprising that the region of stable magnetic moment extends to the region of negative U for a finite J. The key to understand this result is the extension of the formed magnetic moment. Longer correlation length of the Kondo insulator with smaller J means larger spread of the magnetic moment. It means that the effect of Coulomb repulsion (attraction for negative U) is weakened for smaller J. In the weak coupling case, the correlation length diverges exponentially as a function of J. On the other hand, the charge gap which is linear in J [12] acts in the Kondo lattice parts as a positive effective potential.

It is interesting to compare the effects of depletion of localized spins between the two-leg spin ladder and the one dimensional Kondo insulator. The both system have spin gaps as a common feature. For the spin ladder, depletion of a spin always leads to formation of a localized moment around the depleted site. For the Kondo chain, formation of a magnetic moment depends on (U, ϵ).

A finite concentration of depletion may lead to quasi long range order characterized by gap-less spin excitations in the spin ladder. On the other hand for the Kondo insulator, one can speculate that there may be two cases. In one case, the ground state may be non-magnetic, while in the other case there may be quasi long range anti-ferromagnetic ordering. This will be an interesting future problem.

Finally let us consider the effect of non-magnetic impurities in real three dimensional Kondo insulators. We believe that the first conclusion that the formation of magnetic moment is generally easier in Kondo insulators than in ordinary metals is also valid in higher dimensions. It is also probable to consider that there may be the two cases, non-magnetic and magnetic ground states for finite concentrations of non-magnetic impurities in the Kondo insulators in realistic three dimension. However, estimation of the critical concentration for each case needs more elaborate investigation and clearly beyond the range of the present paper.

Acknowledgments

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